Acetamide, 2-(2-thiophenyl)-N-ethyl-N-isobutyl-

Inchi: InChI=1S/C12H19NOS/c1-4-13(9-10(2)3)12(14)8-11-6-5-7-15-11/h5-7,10H,4,8-9H2,1-3H

InchiKey: KPPDNHRRMNKQFD-UHFFFAOYSA-N

Formula: C12H19NOS

SMILES: CCN(CC(C)C)C(=O)Cc1cccs1

Mol. weight [g/mol]: 225.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.65		Crippen Method
logp	2.795		Crippen Method
mcvol	188.380	ml/mol	McGowan Method
rinpol	1935.00		NIST Webbook
rinpol	1935.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415408&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.